Semiclassical Theory of Short Periodic Orbits in Quantum Chaos

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We have developed a semiclassical theory of short periodic orbits to obtain all quantum information of a bounded chaotic Hamiltonian system. If T_1 is the period of the shortest periodic orbit, T_2 the period of the next one and so on, the number $N_{p.o}$ of periodic orbits required in the calculation is such that $T_1 + \cdots + T_{N_{p.o}} \simeq T_H$, with T_H the Heisenberg time. As a result $N_{p.o} \simeq hT_H/\ln(hT_H)$, where h is the topological entropy. For methods related to the trace formula $N_{p.o} \simeq \exp(hT_H)/(hT_H)$.

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The semiclassical evaluation of energy spectra in classically chaotic Hamiltonian systems was started in 1971 with the Gutzwiller's trace formula [1]. From then on a big effort was dedicated to extend the formalism to wave functions [2] and to use resummation techniques to improve convergence properties of trace formulas [3,4]. However, a common drawback in all those approaches is the requirement of an enormous number of periodic orbits (**P.O**s), restricting explicit calculations to very special systems; e.g., systems where classical mechanics is handled by a symbolic dynamics. Moreover, these approaches miss a simple understanding of wave mechanics in terms of classical objects.

Recently it was shown that chaotic eigenfunctions can be described in terms of a small number of localized structures living on short periodic orbits [5]. Having this in mind, we present a simple semiclassical formalism to obtain quantum mechanics from a very small number of short **P.O**s. In order to do so, we will construct resonances (or scar functions) [6] of short **P.O**s explicitly, evaluating the interaction between them.

Let γ be an unstable **P.O** isolated on each energy surface. We introduce a curvilinear coordinate system choosing the x axis along the trajectory and the y axis perpendicular to it at x (to simplify the exposition we take only one transversal direction). On the **P.O** $y=0$. Classical mechanics in a neighborhood of the orbit is governed by a transversal symplectic matrix $M(x)$ of elements $m_{ij}(x)$ $(i,j=1,2)$, which describes the linearized motion on the energy surface. Then, a point with transversal coordinates (y, p_y) at $x=0$ evolves according to the following rule:

$$\begin{pmatrix} y(x) \\ p_y(x) \end{pmatrix} = \begin{pmatrix} m_{11}(x) & m_{12}(x) \\ m_{21}(x) & m_{22}(x) \end{pmatrix} \begin{pmatrix} y \\ p_y \end{pmatrix}.$$

We have selected the origin $x=0$ such that $m_{11}(L) = m_{22}(L)$, with L the length of γ [7]. There are at least 2ν points on the orbit satisfying that condition, with ν the Maslov index. With this choice the monodromy matrix $M(L)$ acquires the form,

$$M(L) = (-1)^\nu \begin{pmatrix} \cosh(\lambda L) & \sinh(\lambda L)/\tan(\varphi) \\ \sinh(\lambda L)\ \tan(\varphi) & \cosh(\lambda L) \end{pmatrix}.$$

λ is the Lyapunov exponent in units of $[length^{-1}]$ and $\tan(\varphi)$ $(\neq 0)$ in units of $[momentum/length]$ defines the slope of the unstable manifold in the plane $y-p_y$ (the slope of the stable manifold being $-\tan(\varphi)$).

In general it is impossible to compare vectors living in the plane $y-p_y$ because the axes have different units. However, when the directions are symmetrical with respect to the axes it is only necessary to compare one component. Then, we change to new axes ξ_u and ξ_s, on the unstable and stable manifolds respectively, such that their projections on each axis are equal in absolute value. The symplectic matrix B transforming coordinates from the new axes into the old ones is

$$B = (\xi_u\ \xi_s) = (1/\sqrt{2}) \begin{pmatrix} 1/\alpha & -s/\alpha \\ s\ \alpha & \alpha \end{pmatrix},$$

with $\alpha = \sqrt{|\tan(\varphi)|}$ and $s = \mathrm{sign}(\varphi)$. Observe that $B^{-1}M(L)B = (-1)^\nu \exp(\lambda L D)$, with D a diagonal matrix of elements $d_{11}=1$ and $d_{22}=-1$.

Now, we decompose $M(x)$ into a periodic matrix $F(x)$ describing the evolution of the manifolds, and a matrix (depending in a simple way of x) describing the exponential contraction-dilation along the manifolds,

$$M(x) = F(x)\ \exp(x\lambda K) \equiv F(x)\ B\ \exp(x\lambda D)\ B^{-1}, \quad (1)$$

with $K \equiv BDB^{-1}$ $[k_{11}=k_{22}=0,\ k_{21}=1/k_{12}=\tan(\varphi)]$. Equation (1) defines $F(x)$ in terms of $M(x)$ and we can see that $F(L) = (-1)^\nu \mathbb{1}$. Floquet's theorem [8] affirms that the decomposition given in (1) can also be obtained for systems with many transversal directions.

Now, it is possible to construct a family of resonances associated to γ. We adapt well known semiclassical techniques to obtain eigenfunctions concentrated in the neighborhood of stable **P.O**s [9]. In the x direction we consider the typical solution of a one dimensional motion, and in the transversal one we use a wave packet which evolves according to $F(x)$,

$$\psi_\gamma(x,y) = \frac{\exp\{i\ [S(x) + y^2\ \Gamma(x)/2]/\hbar - i\ \phi(x)/2\}}{\sqrt{T\ \dot{x}}\ \ [\pi\ (\hbar/J)\ |Q(x)|^2]^{1/4}}, \quad (2)$$

where $S(x) = \int_0^x m\dot{x}\ dx$ is the action, T the period of γ and J the unit area in the plane $y-p_y$. $\Gamma(x) \equiv$

$P(x)/Q(x)$, with $Q(x)$ $[P(x)]$ the y (p_y) component of the complex vector [10]

$$\xi_u(x) + i\,\xi_s(x) \equiv F(x)(\xi_u + i\,\xi_s) = M(x)B \begin{pmatrix} e^{-x\lambda} \\ i\,e^{x\lambda} \end{pmatrix}. \quad (3)$$

Equation (3) shows that it is not necessary to evaluate explicitly $F(x)$. The area preserving property of $F(x)$ guarantees the following normalization condition:

$$Q^*(x)\,P(x) - Q(x)\,P^*(x) = 2i\,\xi_u(x) \wedge \xi_s(x) = 2iJ. \quad (4)$$

Then, $\mathrm{Im}[\Gamma(x)] = J/|Q(x)|^2 > 0$. Accordingly ψ_γ is concentrated around γ and well-behaved in all regions except in the neighborhood of a turning point ($\dot{x} = 0$) [11]. Finally, the complex number $Q(x)$ sweeps an angle $\phi(x)$ while evolving from 0 to x, and $\nu \equiv \phi(L)/\pi$ (this is the definition of the Maslov index).

ψ_γ is a continuous function at $x = L$ if the accumulated phase around the orbit is an integral multiple of 2π. This condition determines the admitted energies E_γ of the **P.O** and corresponds to the Bohr-Sommerfeld quantization rule: $S(L)/\hbar - \nu\pi/2 = 2n\pi$, where $n = 0, 1, \ldots$ is the number of excitations along γ.

We stress that the semiclassical construction of eigenfunctions in the neighborhood of *stable* orbits is similar to (2). The initial complex vector of equation (3) is replaced by the eigenvector of the monodromy matrix (a complex vector in this case) satisfying (4). And of course, the evolution of the vector is given by the transversal symplectic matrix without modifications. Eigenvalues have an error $\mathcal{O}(\hbar)$ and eigenfunctions an error $\mathcal{O}(\sqrt{\hbar})$. Moreover, it is possible to improve the accuracy by including transversal excitations [9].

In our case, there is an essential error because the evolution in (3) is given by a modified transversal matrix. In order to eliminate that error, we will first evaluate the action of the semiclassical evolution operator for infinitesimal times over the resonance in the form

$$\hat{H} \equiv i\hbar\,\lim_{\delta t\to 0}(\hat{U}(\delta t) - \hat{1})/\delta t. \quad (5)$$

The classical transversal evolution from x to $x + \delta x$ is given by $M_x(\delta x) = M(x + \delta x)\ M(x)^{-1}$. So, $M_x(\delta x)\ F(x) = F(x + \delta x)\ \exp(\delta x\ \lambda K)$. Observing that $K\xi_u = \xi_u$ and $K\xi_s = -\xi_s$, it results to first order in δx:

$$\begin{aligned} M_x(\delta x)\ \xi_u(x) &\simeq (1 + \delta x\ \lambda)\ \xi_u(x + \delta x), \\ M_x(\delta x)\ \xi_s(x) &\simeq (1 - \delta x\ \lambda)\ \xi_s(x + \delta x). \end{aligned} \quad (6)$$

The above expressions actually show clearly the approximation involved in the construction. We have forced the vector ξ_u (ξ_s) to evolve without dilation (contraction) while the right evolution dilates (contracts) the vector with a rate specified by λ. Then, we set $\delta x = \dot{x}\ \delta t$ and use (6) to evaluate the action of $\hat{U}(\delta t)$ on ψ_γ. Finally, after some calculations we obtain from (5),

$$\hat{H}\psi_\gamma(x, y) = g_\gamma(x, y)\ \psi_\gamma(x, y), \quad (7)$$

with $g_\gamma(x, y) = E_\gamma + i\hbar\dot{x}\lambda\ (y^2 J/\hbar - |Q(x)|^2/2)/Q(x)^2$.

Then, the application of the semiclassical Hamiltonian operator to the resonance gives the term $E_\gamma\psi_\gamma$ as expected, plus a resonance of γ with two excitations in the transversal direction. In fact, the two excitations are also expected because the right evolution produces a quadrupole-like deformation of the wave packet. Equation (7) is a extremely powerful tool: it is the key to evaluate matrix elements between **P.O**s. As the operator $\hat{H}$ is not exactly Hermitian for finite values of $\hbar$, we define a symmetrized interaction between two **P.O**s γ and δ as follows (in Dirac's notation):

$$\begin{aligned} \langle\delta|\hat{H}|\gamma\rangle &\equiv\ (\langle\delta|\hat{H}\gamma\rangle + \langle\gamma|\hat{H}\delta\rangle^*)/2, \\ \langle\delta|\hat{H}^2|\gamma\rangle &\equiv\ \langle\hat{H}\delta|\hat{H}\gamma\rangle. \end{aligned} \quad (8)$$

By using (7), we obtain explicitly the following diagonal matrix elements in the semiclassical limit $\hbar \to 0$,

$$\begin{aligned} &i)\ \ \langle\gamma|\gamma\rangle \to 1, \\ &ii)\ \ \overline{E}_\gamma \equiv \langle\gamma|\hat{H}|\gamma\rangle/\langle\gamma|\gamma\rangle \to E_\gamma, \\ &iii)\ \ \sigma_\gamma^2 \equiv \langle\gamma|\hat{H}^2|\gamma\rangle/\langle\gamma|\gamma\rangle - \overline{E}_\gamma^2 \to (\hbar\lambda)^2\ \overline{\dot{x}^2}/2, \end{aligned}$$

with $\overline{\dot{x}^2} = S(L)/mT$ the time average of $\dot{x}^2$ on the orbit. Expression *iii)* shows that the width σ_γ of the resonance is asymptoticaly proportional to λ. Moreover, $\rho_E\ \sigma_\gamma = \mathcal{O}(\hbar^{-1})$ [12] shows that a unique orbit cannot support a stationary state in the semiclassical limit (to support an eigenfunction the width of a resonance needs to satisfy $\rho_E\ \sigma < 1$). Of course, this result is well known [13].

We should say some words about symmetry. If the system is time reversal it is easy to show that $\psi_{-\gamma}(x, y) = \psi_\gamma(x, y)^*$ and $\hat{H}\psi_{-\gamma}(x, y) = (\hat{H}\psi_\gamma(x, y))^*$, where $-\gamma$ is the time reversal partner of γ. If the system also includes a spatial symmetry G, it results that $\psi_{G\gamma}(x, y) = G\psi_\gamma(x, y)$ and $\hat{H}\psi_{G\gamma}(x, y) = G\hat{H}\psi_\gamma(x, y)$. So, to obtain real eigenfunctions inside a defined symmetry representation, we construct real resonances inside the same representation by using group theory [14].

For low or medium energies we can evaluate matrix elements directly on the domain; however, for high energies or to obtain explicit expressions in terms of classical quantities as $\hbar$ goes to zero, it is preferable to work on a surface of section [15]. Let ζ be a differentiable curve with the coordinate q along it, and η perpendicular to ζ at q ($\eta = 0$ on the curve). Suppose γ crosses the section at q_j $(j = 1, \ldots, m)$ with angles θ_j; the corresponding positions on γ being x_j (see Fig. 1(a)). In a neighborhood of radio $\mathcal{O}(\sqrt{\hbar})$ around the intersection point j, the coordinates are related to order $\hbar$ by $x - x_j = \sin(\theta_j)\ (q - q_j) - \cos(\theta_j)\ \eta$ and $y = \cos(\theta_j)\ (q - q_j) + \sin(\theta_j)\ \eta$. Then, the restriction of ψ_γ to ζ, up to $\mathcal{O}(\sqrt{\hbar})$, is a sum of wave packets in one dimension with tangential momentum $p_j = m\ \dot{x}_j \sin(\theta_j)$,

$$\varphi_\gamma(q) \equiv \psi_\gamma(x,y)|_\zeta = \sum_{j=1}^{m} \psi_{\gamma_j}(q), \qquad (9)$$

with $\psi_{\gamma_j}(q) = \exp[i\, p_j(q-q_j)/\hbar]\ \psi_\gamma[x_j, \cos(\theta_j)(q-q_j)]$.

If the system is bounded by a hard wall and we take this wall like the Poincaré surface of section, ψ_γ is null there up to order $\sqrt{\hbar}$ [16]. In the neighborhood of a bouncing point, ψ_γ consists of two terms associated to the incoming and outgoing trajectory such that the combination satisfies boundary conditions [9] (see Fig. 1(b)). Then, working with its normal derivative we define

$$\varphi_\gamma(q) \equiv -\frac{i\hbar}{2m}\frac{\partial \psi_\gamma}{\partial \eta}(x,y)|_\zeta = \sum_j \dot{x}_j \cos(\theta_j)\psi_{\gamma_j}(q). \quad (10)$$

Moreover, $\hat{H}\varphi_\gamma(q) \equiv \hat{H}\psi_\gamma(x,y)|_\zeta$ for (9) and $\hat{H}\varphi_\gamma(q) \equiv -(i\hbar/2m)\partial\hat{H}\psi_\gamma/\partial\eta(x,y)|_\zeta$ for (10) are obtained to the leading order from (9) or (10) taking into account that

$$\hat{H}\psi_{\gamma_j}(q) \simeq g_\gamma[x_j, \cos(\theta_j)(q-q_j)]\ \psi_{\gamma_j}(q). \qquad (11)$$

From now on $\varphi_\gamma(q)$ (Eq. (9) or (10)) is the object representing the resonance on the section. In order to describe an effective Hilbert space we define a norm on ζ,

$$\langle\gamma|\gamma\rangle_\zeta \equiv \int_\zeta \varphi_\gamma(q)^*\ \varphi_\gamma(q)\ f(q)\ dq, \qquad (12)$$

such that *i*), *ii*) and *iii*) are satisfied. Then, evaluating the leading term of the integral in (12), it results in a classical criterium for specifying $f(q)$

$$T = \sum_{j=1}^{m} f(q_j)\ [\dot{x}_j\ \cos(\theta_j)]^{\mp 1}. \qquad (13)$$

The signs $(-)$ and $(+)$ correspond to (9) and (10) respectively. We select a smooth real function $f(q)$, oscillating so slowly as possible, which satisfies (13) for all short **P.O**s required in the calculation. We notice that the existence of $f(q)$ is not guaranteed for all sections. A hint to choose a section could be to make sure that the classical motion between consecutive points (the map) is simple. For example, in billiards the motion between bounces with the boundary is simple. On the other hand, eigenfunctions of billiards are reduced to the boundary in terms of their normal derivatives, and the metric on the boundary is defined by setting $f(q) = 2\ (\mathbf{r}.\hat{\mathbf{n}})_{(q)}/\dot{x}^2$ [17], with $\hat{\mathbf{n}}$ the unit outgoing normal to the boundary and $\mathbf{r}$ the position vector. Then, condition (13) (with sign $(+)$) reduces to

$$L = \sum_{j=1}^{m} 2\ (\mathbf{r}.\hat{\mathbf{n}})_{(q_j)} \cos(\theta_j),$$

and this nice identity is valid for any **P.O** in any billiard; the demostration being a simple geometrical problem.

Now we can evaluate matrix elements over the section by using equations (9) or (10), (11) and (12) [δ crosses the section at q_k ($k=1,\ldots,m'$) with angles θ_k],

$$\langle\delta|\hat{O}\gamma\rangle_\zeta = \sum_{j,k=1}^{m,m'} A_{jk} \int_\zeta \psi_{\delta_k}(q)^* \hat{O}\psi_{\gamma_j}(q)\ f(q)\ dq. \qquad (14)$$

$A_{jk} = 1$ for (9) and $A_{jk} = \dot{x}_j\dot{x}_k\cos(\theta_j)\cos(\theta_k)$ for (10). Defining $z_l = -i\cos^2(\theta_l)\Gamma(x_l)/2$, $c_l = q_l + ip_l/2z_l$ and $c_{jk} = (z_j c_j + z_k^* c_k^*)/(z_j + z_k^*)$, the Gaussian integrals in (14) are given by

$$\frac{D_{jk}\ f(c_{jk})\ \exp[-B_{jk}/\hbar + i\ (\alpha_j - \alpha_k)]}{\sqrt{T_\gamma\ T_\delta\ \dot{x}_j\ \dot{x}_k\ |Q(x_j)\ Q(x_k)|\ (z_j + z_k^*)/J}}.$$

$B_{jk} = z_j z_k^*(c_j - c_k^*)^2/(z_j + z_k^*) + p_j^2/4z_j + p_k^2/4z_k^*$ and $\alpha_l = S(x_l)/\hbar - \phi(x_l)/2$. Moreover, $D_{jk} = 1$ for $\hat{O} = \hat{1}$ and $D_{jk} = g_\gamma[x_j, \cos(\theta_j)\sqrt{(c_{jk} - q_j)^2 + \hbar/2(z_j + z_k^*)}]$ for $\hat{O} = \hat{H}$. Then, Eq. (14) gives matrix elements in terms of classical quantities evaluated at the intersection points of the orbits with the surface of section.

Finally, in order to obtain the eigenenergies and eigenfuctions of a bounded chaotic Hamiltonian system in a given energy range, we procced as follows. It is constructed the family of resonances of the shortest periodic orbit γ_1, living in the required energy range. The density of resonances associated to γ_1 is $\rho_1 \simeq T_1/2\pi\hbar$, with T_1 the period of γ_1. Later, we do the same with the next shortest orbit γ_2, and so on (using only primitive orbits). The process stop when the whole density of resonances equals the mean energy density ρ_E,

$$T_H \equiv 2\pi\hbar\ \rho_E \simeq 2\pi\hbar \sum_{k=1}^{N_{p.o}} \rho_k \simeq \sum_{k=1}^{N_{p.o}} T_k. \qquad (15)$$

Equation (15) is actually impressive, it shows that the number of **P.O**s $N_{p.o}$ required in the calculation is very little and increases at most *linearly* with the Heisenberg time T_H. More precisely $N_{p.o} \simeq hT_H/\ln(hT_H)$, where h is the topological entropy. For methods related to the trace formula $N_{p.o} \simeq \exp(hT_H)/(hT_H)$.

Another interesting quantity is the number of resonances N_{res} contributing to one eigenfunction. This number is proportional to the mean dispersion (see *iii*)) and to ρ_E

$$N_{res} \simeq 3.6\hbar\rho_E\ \sqrt{<\lambda^2\ \overline{\dot{x}^2}>}, \qquad (16)$$

with $<\ >$ the average over **P.O**s (using the factor 3.6 in (16), the 99% of an eigenfuntion is recovered). Then, we select N resonances ($N \geq N_{res}$), consecutive in energy, and call them $\Gamma_1, \ldots, \Gamma_N$. Later, by solving the following generalized eigenvalue problem

$$\sum_{j=1}^{N} \left(\langle\Gamma_k|\hat{H}|\Gamma_j\rangle - E\ \langle\Gamma_k|\Gamma_j\rangle\right)\xi_j = 0\ ,\ \ \forall\ k, \qquad (17)$$

the eigenenergies E and eigenvectors ξ in the basis of resonances are given.

The main idea for the selection of resonances is to obtain a quasi-orthogonal basis of highly localized (in

energy) functions. The best way of satisfying quasi-orthogonality is to use short periodic orbits. Now, for orbits with comparable periods we select the one with minimum energy dispersion (see *iii*)). This analysis works for hard chaos systems (where all **P.O**s are unstable and isolated). However, for systems with a fraction of regular motion, we need to include the same fraction of regular functions in the basis. And, for systems with a continuous family of neutral **P.O**s (e.g. the bouncing ball family in the stadium billiard), it is required the corresponding fraction of phase space localized functions.

In conclusion we need to construct adequate functions in each classically different region of phase space, the number of them satisfying the required mean density (obtained semiclassically) in each region. In a chaotic region, functions (we call them resonances) are constructed with the shortest **P.O**s, and the number of them used to fill the Hilbert space is very little as implied in Eq. (15). In order to obtain the interaction between two given short **P.O**s it is possible to follow different strategies. Thinking at classical level it is necessary to use at least a **P.O** living in the neighborhood of the previous ones. Then, to obtain all matrix elements, the period of the orbits required in the full calculation would be of the order of the Heisenberg time, and no advantage is reached with respect to other approaches. However, in this article we showed that thinking at quantum level, the interaction between short **P.O**s can be evaluated simply in terms of transversal excitations. In this way, all the information required in the calculation is contained in short **P.O**s.

We finish with some remarks. i) This theory has been applied successfully to the desymmetrized stadium billiard [18]. ii) In this theory, eigenvalues have an error $\mathcal{O}(\hbar)$ and eigenfunctions an error $\mathcal{O}(\sqrt{\hbar})$. iii) We believe that the inclusion of transversal excitations in the construction of resonances is the way of extending this theory to higher orders in $\hbar$. iv) The basis of resonances is particularly useful for parametric dependent systems. In fact, this is the *diabatic basis*, so difficult to find in chaotic systems [5]. v) The evaluation of σ_γ as a function of n is a simple an efficient semiclassical measure of scars [19]. vi) The phenomenon of chaos-assisted tunnelling can be studied without external parameters [20].

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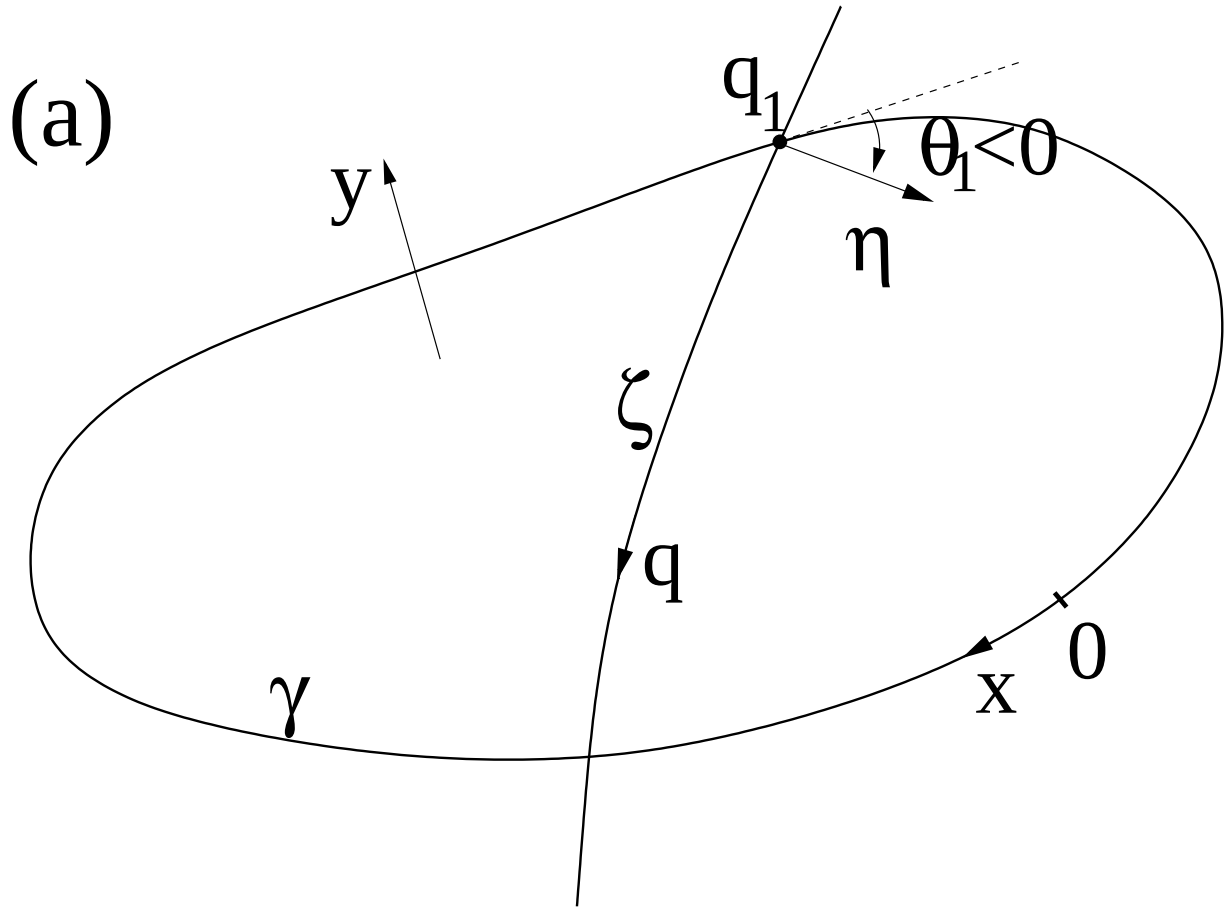
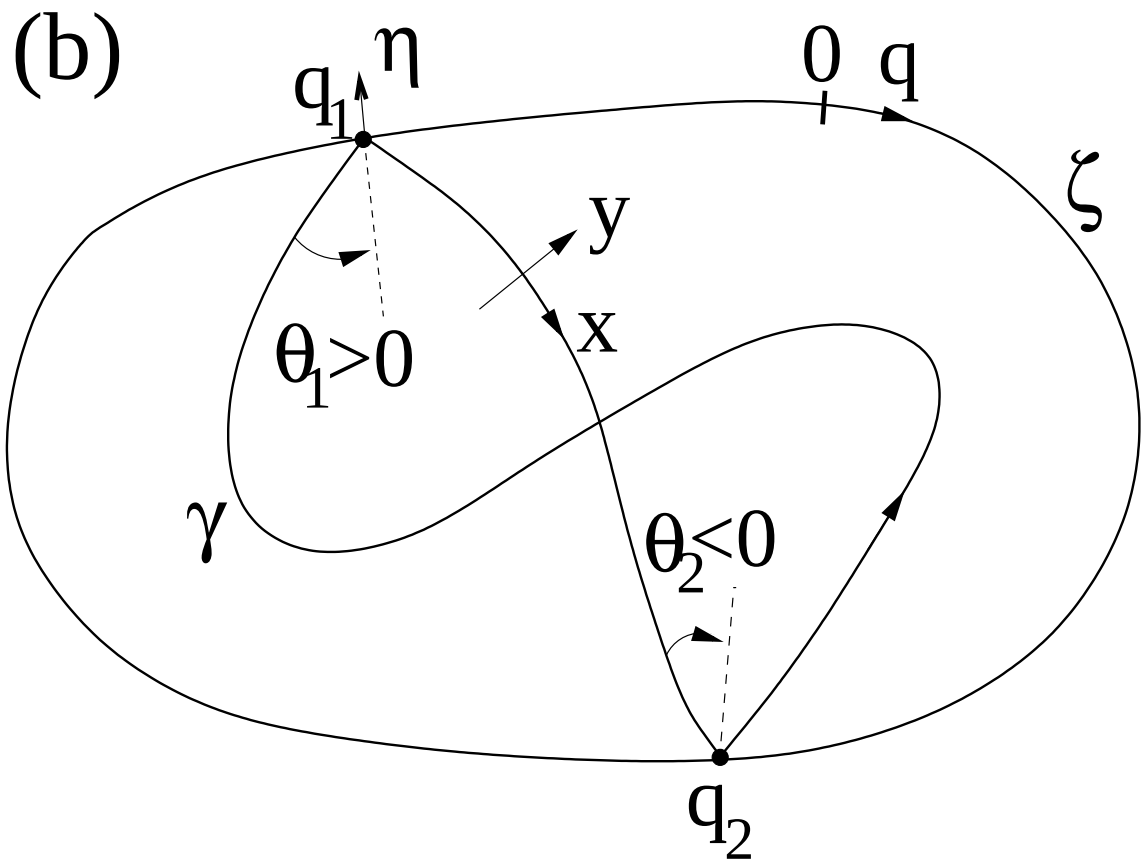
FIG. 1. (a) Coordinates (x, y) and (q, η) defining the neighborhood of the periodic orbit γ and the section ζ respectively. . (b) Idem (a) but the section is given by a hard wall.


(a)
q1
θ1<0
y
η
ζ
q
γ
x
0


(b)
η
q1
0
q
ζ
y
x
θ1>0
γ
θ2<0
q2